

2-Methylheptane
592-27-8 | DTXSID2060460

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.85

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

Image not found

Octane

Measured: 5.18

Predicted: 5.05

Image not found

Ethylcyclohexane

Measured: 4.56

Predicted: 4.45

Image not found

Heptane, 1-chloro-

Measured: 4.15

Predicted: 4.21

Image not found

Nonane

Measured: 5.65

Predicted: 5.44

Image not found

Heptane

Measured: 4.66

Predicted: 4.56